Supporting Information for

Vibrational Sum Frequency Spectroscopic Investigation of the Structure and Azimuthal Anisotropy of Propynyl-Terminated Si(111) Surfaces

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TABLES USED FOR DATA FITTING

Table S1. Fitting Parameters for the Rotational Anisotropy in the Resonant Amplitudes of the PPP Spectra.

As prepared CH_3CC–Si(111) samples			
	A (a.u.)	C (a.u.)	ϕ_0 (deg)
CH_3 r^+	0.014	0.286	104.94
CH_3 r^-	0.103	0.300	84.520
Annealed CH_3CC–Si(111) samples			
	A (a.u.)	C (a.u.)	ϕ_0 (deg)
CH_3 r^+	0.009	0.033	75.463
CH_3 r^-	0.024	0.500	80.905

Table S2. Fitting Parameters for PPP Spectra for as-prepared CH_3CC–Si(111) Samples.

Rotation	A_{NR}	ϕ	B_1	Γ_1	ω_1	B_2	Γ_2	ω_2	B_3	Γ_3	ω_3
Angle (deg)	(a.u.)	ϕ	(a.u.)	(cm^{-1})	(cm^{-1})	(a.u.)	(cm^{-1})	(cm^{-1})	(a.u.)	(cm^{-1})	(cm^{-1})
0	–0.006	0.6	0.3	11.1	2869.7	0.5	15.5	2930.8	0.3	13.5	2958.5
30	–0.003	0.1	0.3	10.7	2867.7	0.4	13.7	2928.2	0.2	11.8	2954.9
60	–0.002	0.5	0.3	10.6	2868.3	0.4	14.1	2928.7	0.3	13.6	2956.9
90	–0.005	0.9	0.2	10.9	2870.0	0.3	13.8	2931.6	0.3	14.7	2961.5
120	–0.005	0.9	0.2	10.9	2870.0	0.3	13.7	2931.6	0.3	14.7	2961.5
150	–0.008	1.0	0.3	11.5	2870.0	0.4	14.7	2931.6	0.2	12.4	2958.7
180	–0.004	0.8	0.3	11.2	2870.0	0.4	14.7	2931.9	0.3	14.4	2960.8
210	–0.005	1.5	0.3	10.2	2869.7	0.4	15.0	2929.9	0.4	16.8	2960.0
240	–0.004	0.5	0.3	11.4	2868.1	0.4	15.3	2928.7	0.3	13.6	2957.2
270	–0.014	1.1	0.3	11.6	2867.0	0.4	15.0	2928.5	0.2	11.7	2955.5
300	–0.005	0.5	0.3	11.5	2869.4	0.5	15.8	2930.2	0.3	14.2	2959.1
330	–0.002	1.5	0.3	11.3	2870.0	0.4	14.5	2932.0	0.4	16.0	2961.6
360	–0.007	1.0	0.3	11.7	2870.0	0.4	15.2	2932.0	0.3	14.3	2960.9

Table S3. Fitting Parameters for PPP Spectra for CH_3CC–Si(111) Samples Annealed at 320 °C Under Vacuum.[a]

Rotation	A_{NR}	ϕ	B_1	Γ_1	ω_1	B_4	Γ_4	ω_4
Angle (deg)	(a.u.) × 10^{-4}	ϕ	(a.u.) × 10^{-2}	(cm^{-1})	(cm^{-1})	(a.u.) × 10^{-2}	(cm^{-1})	(cm^{-1})
0	4.4	2.1	4.1	11.1	2878.0	6.0	12.3	2972.6
10	8.3	3.5	4.0	11.5	2878.0	4.3	10.8	2971.7
20	14	0.8	3.9	11.4	2877.1	3.2	9.7	2970.3
30	25	1.1	3.1	11.2	2875.9	2.4	9.2	2970.4
40	27	1.1	2.8	11.2	2875.9	2.3	9.2	2971.1
50	12	0.8	3.2	11.2	2877.2	3.5	10.4	2971.5
60	10	–1.0	5.8	12.8	2877.1	6.3	12.2	2973.1
70	9.4	1.6	3.5	11.8	2878.0	6.1	12.2	2971.6
80	14	1.1	3.7	12.6	2878.0	6.2	11.7	2971.3
90	18	1.0	3.4	11.7	2877.9	6.3	11.6	2971.0
100	17	1.1	3.3	11.5	2878.0	6.5	11.7	2971.0
110	13	1.3	3.4	12.5	2877.9	6.4	11.5	2971.7
120	8.3	1.9	2.9	11.1	2877.3	6.1	11.5	2972.1
130	8.6	3.6	2.8	11.4	2874.9	4.4	10.3	2972.2
140	23	-2.1	2.2	10.7	2873.3	3.1	9.6	2972.1
150	42	1.1	1.6	10.3	2871.9	2.0	8.7	2971.3
160	38	1.2	1.8	10.7	2871.7	2.2	8.8	2971.3
170	24	1.1	2.2	11.8	2872.1	2.7	9.1	2972.5
180	6.2	0.8	2.4	10.6	2875.9	5.3	10.8	2971.9
190	12	1.5	3.3	11.6	2878.0	6.2	11.8	2971.6
200	15	1.1	3.1	9.5	2876.0	6.0	11.4	2971.7
210	20	1.0	3.8	10.9	2878.0	6.5	12.2	2970.6
220	18	1.0	4.2	11.9	2878.0	6.5	12.2	2970.9
230	17	1.1	3.3	11.5	2878.0	6.5	11.7	2971.0
240	4.9	2.2	3.9	12.1	2878.0	5.6	12.1	2972.3
250	8.6	3.6	3.8	12.1	2877.3	4.4	11.0	2971.3
260	28	1.1	2.7	11.3	2875.0	2.4	9.5	2971.7
270	3.9	1.0	2.8	12.4	2875.1	2.7	11.5	2971.3
280	32	1.1	2.7	11.7	2874.8	2.1	9.4	2970.8
290	15	0.8	3.6	11.7	2876.5	3.5	10.3	2971.2
300	5.9	6.0	4.3	12.7	2877.4	4.9	11.6	2971.8
315	15	1.4	5.1	11.4	2878.0	7.8	13.3	2971.4
330	19	1.1	4.5	10.8	2878.0	6.6	12.3	2970.7
340	19	1.2	5.0	11.0	2878.0	7.7	13.4	2970.8
350	13	1.4	5.0	11.5	2878.0	7.4	12.9	2971.5
360	5.9	6.0	4.3	12.7	2877.4	4.9	11.6	2971.8

[a]Only values for the C–H symmetric and asymmetric stretches are given.